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Some remarks on the electronic states in disordered materials

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Abstract. In this paper we recall how the field theory formalism is very useful for computing the density of electronic levels in disordered materials, and we stress those characteristics of the associated field theory which are peculiar to this model. In particular, we show that the localisation transition associated with the mobility edge has rather strange properties from the point of view of pure field theory: a sound computation of the critical exponents associated with the mobility edge is rather difficult, due to this unusual behaviour.

1. Introduction

Since the first paper by Anderson (1958) on localisation of electrons, a lot of work has been done on the electronic structure of amorphous materials (for a review see Thouless (1974, 1978)). If one neglects the electron–electron interaction, the problem is reduced to the computation of the levels of the Schrödinger operator

$$H_R = -\Delta + V(x), \tag{1}$$

where $V(x)$ is a random potential dependent on the atomic structure of the material, and Δ is the D-dimensional Laplacian. In the simplest approach one studies only the case where $V(x)$ is a white noise, i.e. where it has a Gaussian distribution with covariance

$$\overline{V(x)V(y)} = g\delta^D(x-y), \tag{2}$$

where g plays the role of coupling constant. In the rest of this paper we will consider only this case.

The goal consists of computing the Green functions of the operator H_R from the mean over the random potential $V(x)$. From the knowledge of the Green functions, one can extract physically interesting information such as the density of states, the conductivity of the system and the nature of the electronic states (localised or extended states).

A possible approach to this problem consists of mapping it onto the problem of computing the Green functions of an appropriate field theory. This approach has been very successful, especially for the computation of the density of states; unfortunately less progress has been made in studying the behaviour of the conductivity near the mobility edge which separates localised from extended states. Indeed, the localisation transition, which is the field theoretical equivalent of the mobility edge, has rather unique characteristics which are not shared by any 'real' transition. Most of the troubles

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are due to the fact that the equivalent model of field theory is not a true field theory, but is the analytic continuation in a parameter of a *bona fide* field theory: in performing the analytic continuation, most of the physical intuition we have gathered may be lost (especially inequalities coming from positivity), and rather paradoxical situations can be reached. (This happens in the theory of spin glasses: see Parisi (1979, 1980).)

The aim of this paper is to underline these difficulties and to stress the points in which the localisation transition differs from a normal transition.

In § 2 we review the general field theoretical formalism we use, while in § 3 we show how this formalism can be successfully used to compute the density of levels. In § 4 we study the appropriate perturbative expansion for the conductivity and see how long-range correlations are present in the conducting phase. In the last section we discuss and present the results obtained in the previous sections.

2. The field theory formalism

We want a representation for the following quantities:

$$G_R(x-y)=\overline{G^V(x,y)}, \qquad |G|^2_R(x-y)=\overline{|G^V(x,y)|^2},$$
$$G^V(x,y)=\langle x|(H_R-E)^{-1}|y\rangle, \tag{3}$$

where the bar denotes the mean over the random potential V.

From the knowledge of these, one can compute the density of states ρ and the conductivity σ, e.g.

$$\rho = \operatorname{Im} G_R(0)/\pi. \tag{4}$$

To this end we must consider the O(N) invariant Lagrangian:

$$\mathscr{L}(x)=\sum_{i=1}^{N}[(\partial_\mu\phi_i)^2-E\phi_i^2]-g\Big(\sum_{i=1}^{N}\phi_i^2\Big)^2 \tag{5}$$

where ϕ_i are N-component fields. The generating functional of the correlation functions of the field ϕ is given by

$$Z\{J\}\propto\int \mathrm{d}[\phi]\exp\Big[-\int \mathrm{d}x\Big(\mathscr{L}(x)+\sum_{i=1}^{N}J_i(x)\phi_i(x)\Big)\Big]. \tag{6}$$

Using symmetry arguments, one finds that the two-field correlation function satisfies the relation (Economou and Cohen 1970, Nitzan *et al* 1977, Thouless 1975, Aharony and Imry 1977, Edwards 1979)

$$\langle\phi_i(x)\phi_j(y)\rangle = G(x-y)\delta_{i,j}. \tag{7}$$

The theory (in particular $G(x)$) is well defined for any integer value of N; an analytic continuation in N to non-integer values can be made: for $N=0$ one finds that

$$G_R(x)=G(x). \tag{8}$$

This result is very useful because it allows us to use the whole technology developed in the study of standard field theory, in particular the Feynman diagrammatic expansion and the renormalisation group.

In the same spirit one can introduce the Lagrangian

$$\mathscr{L}(x)=\sum_{i=1}^{N}[(\partial_\mu\phi_i^+)^2+(\partial_\mu\phi_i^-)^2-E(\phi_i^+)^2-\bar{E}(\phi_i^-)^2]-g\Big(\sum_{i=1}^{N}[(\phi_i^+)^2+(\phi_i^-)^2]^2\Big). \tag{9}$$

E is *a priori* a complex parameter and $\bar{E}$ denotes its complex conjugate. In the limit $n\to 0$ the correlation functions of the field ϕ^+ are identical to those of the field ϕ; moreover one finds that

$$\begin{aligned}&\langle\phi_i^+(x)\phi_k^+(y)\rangle=\overline{\langle\phi_i^-(x)\phi_k^-(y)\rangle},\\&\sum_{i=1}^{N}\langle\phi_k^+(x)\phi_j^-(x)\phi_i^+(y)\phi_i^-(y)\rangle=\delta_{kj}|G|_{\mathrm{R}}^2(x-y).\end{aligned} \tag{10}$$

The Green function $|G|_{\mathrm{R}}^2(x)$ is needed to study the presence of localised states: one expects that, if and only if localised states are present, the function $|\psi|_{\mathrm{R}}^2(x)$ defined by

$$\lim_{\mathrm{Im}E\to 0}|G|_{\mathrm{R}}^2(x)\,\mathrm{Im}\,E=|\psi|_{\mathrm{R}}^2(x) \tag{11}$$

is non-trivial: $|\psi|_{\mathrm{R}}^2(x)$ represents the square of the wavefunction of the localised states.

The transition, as a function of the energy, from extended to localised states is characterised by the divergence of the correlation functions in the configuration space. This divergence, which is foreign to all the tradition in field theory, is possible here also because the functional integral in equation (6) is not well defined as it stands (the coupling constant has the wrong sign!) and it can be defined only after a rotation of the path of integration in the functional space.

Let us present an example, which will be useful later, of the way in which a well known relation can be obtained in this formalism. We start from the relation

$$\frac{1}{H_{\mathrm{R}}-E}-\frac{1}{H_{\mathrm{R}}-\bar{E}}=\frac{-2\,\mathrm{Im}\,E}{(H_{\mathrm{R}}-E)(H_{\mathrm{R}}-\bar{E})}. \tag{12}$$

If we bracket it with $\langle x||x\rangle$ and use the completeness of the states, we find

$$G^V(x,x|E)-G^V(XX|\bar{E})=-2\,\mathrm{Im}\,E\int G^V(x,y|E)G^V(y,x|\bar{E})\,\mathrm{d}^Dy \tag{13}$$

where we have written explicitly the dependence on the energy (E) of the Green functions (this was implicit in equation (3)). After the integration over the random field V, we obtain (Velicky 1969)

$$G_{\mathrm{R}}(0|E)-\overline{G_{\mathrm{R}}(0|E)}=-2\,\mathrm{Im}\,E\int|G|_{\mathrm{R}}^2(y)\,\mathrm{d}^Dy. \tag{14}$$

How do we recover equation (4)? If $\mathrm{Im}\,E=0$ the Lagrangian (9) would be invariant under a global O(2) transformation†, its infinitesimal form being

$$\delta\phi^+(x)=\phi^-(x),\qquad \delta\phi^-(x)=-\phi^+(x). \tag{15}$$

It is now a simple exercise in functional integral representations to derive the Ward identity relation in the presence of a symmetry breaking term (Jona-Lasinio 1964,

† After this paper had been completed, a paper was published (Wegner 1979) in which equation (14) was derived from the Ward identities of the O(2) symmetry. However, the conclusions of this paper on the behaviour of the mobility edge are different from ours.

Parisi and Testa 1970). In this particular instance the symmetry breaking term is

$$\sum_{i=1}^{N} \int [(\phi_i^+(y))^2 - (\phi_i^-(y))^2] \, \mathrm{d}^D y \tag{16}$$

and one of the corresponding Ward identities is

$$\langle \phi_k^+(x)\phi_j^+(z)\rangle - \langle \phi_k^-(x)\phi_j^-(z)\rangle = -2 \operatorname{Im} E \sum_{i=1}^{N} \int \langle \phi_k^+(x)\phi_j^-(z)\phi_i^+(y)\phi_i^-(y)\rangle \, \mathrm{d}y. \tag{17}$$

Using the relations (7)–(10), equation (14) follows from equation (17). If the density of states $\rho(E)$ is different from zero, as happens for all possible real values of the energy, the O(2) symmetry is spontaneously broken and the integral in the RHS of equation (4) is divergent, signalling the presence of long-range correlations, which may manifest themselves with a Goldstone boson. In reality (but we are not going to use this observation) the full symmetry group for $\operatorname{Im} E = 0$ is $O(2N)$, which breaks down to $O(N) \times O(N)$: the group which is spontaneously broken is larger than O(2), at least for N greater than 1.

3. The density of levels

Let us consider the Lagrangian (6); using the standard Feynman diagram technique, the Green functions can be expanded in series of the coupling constant g. No problems arise in perturbation theory when E is negative (positive mass). When E is positive, the mass in the Lagrangian becomes negative: in a conventional field theory one would shift the field in order to obtain a positive renormalised mass; here, nothing of this kind happens, and the Green functions for positive E are computed as an analytic continuation from negative E. The final Green functions are no longer real: their imaginary part is connected to the density of states of H_R. Using this technique, one finds

$$\rho(E) = E^{(D-2)/2} F(gE^{(D-4)/2})\theta(E). \tag{18}$$

Equation (18) is correct only if we take care of a finite number of orders of the perturbative expansion. The effect of mass renormalisation would shift the value E_c which separates the two regions where $\rho(E) = 0$ and $\rho(E) \neq 0$ respectively. Equation (18) should be replaced by

$$\rho(E) = \operatorname{Im}(E_c - E)^{(D-2)/2} F[g(E - E_c)^{(D-4)/2}]. \tag{19}$$

The first non-trivial problem consists of computing the behaviour of $\rho(E)$ near E_c. As we shall see later, the situation is more complex and the solution of this problem is irrelevant to physics.

In the coherent phase approximation (CPA) (Soven 1967, Elliot *et al* 1974), one finds for negative E that the Fourier transform $G(p)$ of $G(x)$ satisfies

$$G(p) = 1/(p^2 + m^2), \qquad -E = m^2 - g(m^{D-2} - \Lambda^{D-2}), \tag{20}$$

where Λ is a cut-off at large frequencies (if the Laplacian is written as a finite difference operator on a lattice with spacing a (see Thouless and Elzain 1978) $\Lambda \propto a^{-1}$), and we have neglected all the proportionality factors.

As is well known, the solution of equation (20) gives

$$\rho \sim (E - E_c)^{\alpha} \theta(E - E_c) \qquad (\alpha = \tfrac{1}{2}) \tag{21}$$

for $E \sim E_c$. The sign of g is crucial. Now when can equation (21) be trusted? At the transition point, m^2 remains different from zero; however, the propagator

$$G_{\phi^2}(K) = \int d^D K \langle \phi^2 \phi^2 \rangle \tag{22}$$

has a pole at $K^2 = 0$, corresponding to a zero-mass bound state. Indeed, in field theory language the ϕ^4 interaction is attractive and not repulsive as usual: a two-particle bound state is produced and by decreasing the mass of the particles (m^2), the mass of the bound state becomes zero when $m^2 \neq 0$. The only infrared singularities are produced by the self interactions of this bound state. This problem can be easily studied using the standard machinery (Aharony and Imry 1977): one introduces a field $q_{ij} = \phi_i \phi_j$ and derives an effective Lagrangian for the field q_{ij}; an interaction proportional to q^3 is present, strongly suggesting that equation (21) holds only for $D > D_S = 6$ and that α can be expanded in powers of $\epsilon = D_S - D$ when $D < D_S$. Some explicit work is needed to verify that there are no difficulties which would forbid the realisation of this program, in particular if D_S is equal to 6, and not to 8, as happens in some polymer systems (Lubensky and Isaacson 1978).

We do not enter into details because this problem is purely academic. Indeed, the unconventional sign of the coupling constant in equation (6) makes the Lagrangian unbounded from below also for $E < 0$. As a consequence, the perturbative expansion cannot be Borel summed, and the Green functions have an imaginary part proportional to $\exp(-1/g)$ also for $E < 0$. This imaginary part can be computed semiclassically (Thouless and Elzain 1978, Cardy 1978), following the pioneering work of Zittartz and Langer (1966), Halperin and Lax (1966, 1967). This effect will give an imaginary part to E_c, shifting it in the second sheet; the singularity at E_c becomes an unphysical one and has a small influence on the 'observable' behaviour of $\rho(E)$ for real E. This last quantity can be easily computed by matching the small coupling expansion with the non-perturbative results proportional to $\exp(-1/g)$. The first computation in this direction has been done by Thouless and Elzain (1978). In recent years much progress has been made in the understanding of the mutual relations between large-order behaviour of the perturbative expansion, the semiclassical non-perturbative contributions and the singularities of the Borel transform with respect to the coupling constant (for a review, see Parisi (1977), Zinn-Justin (1977)); consequently, the matching of the two expansions can be done with good precision (the results for the prefactor can be found in Brézin and Parisi (1980)). It seems that, if no unforeseen difficulties are present, the computation of $\rho(E)$ at all the energies should be more or less straightforward. This is in contrast with the situation concerning localised states, as we will see in the next section.

4. The conducting phase

Let us study the Lagrangian (9). It is believed that for real E two regimes are possible: for E less than E_L only localised states are present, while for $E > E_L$ the states are extended and the conductivity σ is different from zero; we recall that the conductivity is given by the Kubo–Greenwood formula (Edwards 1958)

$$\sigma = \lim_{\epsilon \to 0} \epsilon^2 \int d^D x \, x^2 |G^2|_R(x), \qquad \text{Im } E = \epsilon. \tag{23}$$

At zero order in perturbation theory ($g = 0$)

$$|G^2|_R(x) \sim (1/x^{D-1}) \exp(-\epsilon|x|), \tag{24}$$

and the conductivity σ is infinite, as it should be, in the absence of impurities. The presence of long-range correlations implies that perturbation theory should be used with caution, especially at low momenta.

In the language of relativistic field theory, the long-range behaviour $|G^2|_R(x)$ is due to a pinching singularity at small k when ϵ becomes zero. Indeed, the Fourier transform $|\tilde{G}|^2_R(K)$ is given by

$$|\tilde{G}|^2_R(K) = \int \frac{d^D p}{[(K+p)^2 - E][p^2 - \bar{E}]}$$

$$= \int d^D p \, G(K+p)\bar{G}(p). \tag{25}$$

In other words, when $\epsilon \to 0$, pinching diagrams are the substitute of zero-mass particles. When g is different from zero, the Green function G becomes imaginary (Im $m^2 \neq 0$) and the pinching diagrams, although dominant, do not correspond any more to long-range correlations; however, the Ward identity (17) implies that

$$|G|^2_R(0) \propto \rho(E)/\epsilon. \tag{26}$$

If the function $|G|^2_R(K)$ is not divergent in the limit $\epsilon \to 0$ at $K \neq 0$, equation (26) implies the presence of long-range correlations for $\epsilon \to 0$. In this case one would expect that

$$|\tilde{G}|^2_R(K) \propto 1/K^2 \qquad \text{for } \epsilon = 0 \tag{27}$$

as normally happens in theories with spontaneously broken symmetries.

One must be rather careful in choosing a perturbative expansion in this phase. It is well known that the standard g expansion cannot be used (Langer and Neal 1966): the behaviour of $|\tilde{G}|^2_R(K)$ changes from $1/K$ at $g = 0$ to $1/K^2$ at $g \neq 0$.

The presence of this g-dependent crossover region in momentum space induces infrared divergences in the standard perturbative expansion, i.e. the final result will not be a C^∞ function of g.

Also, if we take care of this effect, the very presence of long-range correlations may produce infrared divergences if $D < 4$. However, the long-range correlations are connected to the spontaneous breakdown of the O(2) symmetry. The Ward identities tell us that these modes decouple in the low-momenta region (Adler's zeros) (for a review see Adler and Dashen (1968)), and they do not contribute to infrared divergences as far as $D > 2$ (this is the well known situation for Heisenberg ferromagnets (Brézin and Zinn-Justin 1976)); equation (27) now becomes

$$|G|^2_R \propto 1/K^2 + 1/K^D. \tag{28}$$

It is clear that finite results may be obtained only if we take care simultaneously of all the Ward identities of the theory and of the presence of two different regimes at small K for $g = 0$ and $g \neq 0$.

We do not want to discuss how this expansion may be realised. This is a technical problem which can be studied using one of the many field theoretical techniques we have at our disposal. The real unsolved problem consists in controlling the situation for $D = 2$. Wegner (1979) suggests that the usual theorems on absence of spontaneous

symmetry breaking imply that the O(2) Goldstone modes must be absent. How can this happen when $\rho(E) \neq 0$? The only possibility would be that

$$\lim_{\epsilon \to 0} \epsilon |\tilde{G}|^2_{\mathrm{R}}(K) \neq 0 \qquad \text{for } K \neq 0. \tag{29}$$

The divergence of equation (26) would not imply a singularity at $K = 0$.

It is usually believed that if equation (29) holds, the states are localised and the conductivity is equal to 0. Following Wegner, we would conclude that for $D = 2$ the states are always localised, as has been suggested by other authors on different grounds.

However, we must always remember that our field theory is only an analytic continuation of a *bona fide* field theory, and one should be very careful in performing analytic continuations of inequalities.

For example, if we consider a spin model, invariant under the group O(N), there is a transition where the symmetry breaks down to O($N-1$), the number of Goldstone bosons is $N-1$ and one would argue that in two dimensions a transition of conventional type would be possible only for $N = 1$. However, we know that for $N = 0$ the spin model corresponds to the self-avoiding walk (de Gennes 1972) which possesses no anomalous behaviour in $D = 2$, although -1 Goldstone bosons would be present below the transition†.

Now it is believed that in any dimensions, for large negative E, all the states contributing to ρ are localised and equation (29) holds. This result is confirmed by explicit computations (Cardy 1978), performed using the semiclassical approach, in which one finds that, for large negative E,

$$|\tilde{G}|^2_{\mathrm{R}}(K) \sim |\psi|^2_{\mathrm{R}}(K)/\epsilon^{(1+N/2)}, \qquad -2 < N < 2. \tag{30}$$

Whereas equation (30) holds also for $N \neq 0$, equation (29) may be satisfied only if $N = 0$. In these semiclassical computations the factors $1/\epsilon$ arise from the integration over the collective coordinates of the instanton in the group space, or in the language of Zittartz and Langer as a pinching contribution in the collective coordinates.

More precisely, if one takes care of the correct complex integration path in functional space, the O(2) group looks more like the O(1, 1) group, i.e. a non-compact group. The integration over this non-compact group gives the terms divergent when $\epsilon \to 0$, i.e. the integration is damped by the terms proportional to ϵ. Indeed, the divergence of the Green functions below E_{L} is a new phenomenon in field theory, and is connected to the presence of this non-compact symmetry group.

If equation (29) holds for $E < E_{\mathrm{L}}$, the absence of conduction for a two-dimensional system would imply that

$$E_{\mathrm{L}} \to +\infty \qquad \text{if } D \to 2. \tag{31}$$

E_{L} denotes the mobility edge and we expect that

$$\sigma \sim (E - E_{\mathrm{L}})^{\gamma}.$$

Unfortunately there is no known method of computing γ.

If we work in perturbation theory in g, $E_{\mathrm{L}} = E_{\mathrm{c}}$ and the critical exponents γ, α, etc., can be easily computed. In this scheme $\rho(E) = 0$, $E < E_{\mathrm{L}}$, i.e. no state, localised or extended, is present for $E < E_{\mathrm{c}}$.

† The author thanks des Cloizeaux and Sourlas for enlightening discussions on this point.

Including the effect of semiclassical configurations, one would obtain $E_c - E_L \sim \exp(-1/g)$, and the exponent γ is fixed by the behaviour in the region where the semiclassical configurations are important.

Long-range correlations, Goldstone bosons, semiclassical configurations and the $n = 0$ limit are all crucial ingredients for understanding the localisation transition, and one should take care of all of them together. It is still an open problem to understand how this can be done, in particular if in higher-dimensional spaces the system simplifies and γ can be computed exactly.

In order to underline those difficulties, which are peculiar to this problem, it is useful (following Nitzan *et al* 1977) to introduce the fields

$$\psi_a^1 = \exp(i\pi/4)\phi_a^1, \qquad \psi_a^2 = \exp(-i\pi/4)\phi_a^2. \tag{32}$$

The Lagrangian (10) now becomes

$$\tfrac{1}{2} i \sum_{a=1}^{N} [(\partial_\mu \psi_a^1) + E(\psi_a^1)^2 - (\partial_\mu \psi_a^2)^2 - E(\psi_a^2)^2] - \tfrac{1}{2} \sum_{a=1}^{N} [(\psi_a^1)^2 + (\psi_a^2)^2] + g\Big(\sum_{a=1}^{N} [(\psi_a^1)^2 - (\psi_a^2)^2] \Big)^2. \tag{33}$$

The corresponding functional integral is now convergent for $\epsilon > 0$: the introduction of the fields ψ^1 and ψ^2 corresponds to fixing the correct integration path in functional space. Apart from the imaginary factor in front of the kinetical term, (33) looks like a conventional Lagrangian; however, in the limit $\epsilon \to 0$, it becomes invariant under the $O(N, N)$ group, i.e. the group of linear transformations on $2N$-dimensional space which leave invariant the form

$$\sum_{a=1}^{N} [(\psi_a^1)^2 - (\psi_a^2)^2].$$

As mentioned before, the $O(N, N)$ group contains as a subgroup, for $N \geqslant 1$, the group $O(1, 1)$, i.e. the two-dimensional Lorentz group.

We face the problem of the restoration of the $O(N, N)$ symmetry which is spontaneously broken in the conducting phase. If the symmetry is unbroken, some of the Green function will diverge when $\epsilon \to 0$ as a consequence of the non-compactness of the symmetry group: an infinite contribution comes from the integration region where $(\psi^1)^2$ and $(\psi^2)^2$ are both large, but $(\psi^1)^2 - (\psi^2)^2$ remains small. The contribution of this integration region is clearly depressed for $\epsilon > 0$.

In other words, the necessity of performing a contour rotation in order to define the integrals for negative g transforms the symmetry group from $O(2N)$ to $O(N, N)$ and the non-compactness of the symmetry group is the origin of the pathologies of the model (e.g. the divergences of the Green functions for $\epsilon \to 0$); of course, the unusual properties of the $O(2N)$ and $O(N, N)$ groups, in the limit $N \to 0$, also contribute to the peculiar properties of the localisation transition.

In order to get a deeper insight into the problem, it is convenient to introduce the fields

$$Q_{a,b}^{i,K} = \psi_a^i \psi_b^K, \qquad i, K = 1, 2, \quad a, b = 1, N,$$

transforming under the tensor representation of the $O(N, N)$ group, and to use the standard methods to derive an effective Lagrangian for the fields $Q_{a,b}^{i,K}$. One could try to investigate the behaviour of the system near two dimensions, by studying if and how the

arguments of Wegner (1979) must be modified; alternatively, one could write down the most general cubic effective Lagrangian and try to use the standard machinery of the renormalisation group to study the critical behaviour near six dimensions.

Both approaches seem quite promising, but they go beyond the aim of this paper, i.e. to underline the peculiarities that the localisation transition acquires when we try to describe it in field theoretical language.

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